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SEMI ANNUAL STATUS REPORT TO

THE NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

N64 81568 *
Code None
(NASA Grant)

T — RESEARCH IN MOLECULAR PHYSICS (NsG-263-63)

For the Period June 1 - November 30, 1963

(NASA CR- - - - )

Submitted by

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Austin 12, Texas

28 Feb. 1964 4p
2258192

February 28, 1964

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MATERIAL PUBLISHED SINCE LAST REPORT

1. C. W. Scherr and Milos Machacek, "Isotope Shifts in the $2^1P$ and $2^3P$ He and $Li^+$ System," JCP 39, 3151 (1963).
2. P. N. Reagan, J. C. Browne and F. A. Matsen, "Dissociation Energy of $He_2^+(^2\Sigma_u^+)$," Phys. Rev. 132, 304 (1963).
3. R. D. Poshusta and F. A. Matsen, "Potential Curve of the Metastable Helium Molecule," Phys. Rev. 132, 307 (1963).

MATERIAL IN PRESS

1. C. W. Scherr and R. E. Knight, "A Remark on the Configuration Interaction Approach," accepted by JCP.
2. C. W. Scherr and R. E. Knight, "Two-Electron Atoms IV. Sixth-Order Expectation Values of Certain Operators of the Ground State," accepted by JCP.
3. F. A. Matsen and J. C. Browne, "Rydberg Orbitals and Energies for $H_2$," accepted as a contribution to the Mulliken Memorial Volume. To be published in MOLECULAR ORBITALS IN CHEMISTRY, Pullman and Lowdin, editors.
4. F. A. Matsen, "Spin-Free Quantum Chemistry," issued as a technical report. To be published in Volume I, ADVANCES

IN QUANTUM CHEMISTRY, P. O. Lowdin, editor.

5. F. A. Matsen, "Spin-Free Quantum Chemistry II. Three-Electron Systems," submitted to JCP.
6. J. C. Browne, "Some Excited States of the Hydrogen Molecule. I. $^1\Pi_u(1s2p\pi)$ and $^3\Pi_u(1s2p\pi)$," submitted to JCP.

MATERIAL IN PREPARATION

1. C. W. Scherr and Milos Machacek, "The P States of Systems of Three Coulombic Particles."
2. C. Sanders, Milos Machacek and C. W. Scherr, "A True Mass Study of the Helium Atom I. The $2^1P$ State."
3. J. C. Browne, "Some Excited States of $He_2^{++}$."
4. J. C. Browne, "Some Excited States of the Helium Molecule: $^1\Sigma_u$ and $^1\Sigma_g$."
5. Judy Hempel, J. C. Browne and F. A. Matsen, "Rydberg States of Li." This is an extension of our work on $H_2$ and involves no new principles.
6. Lawrence Ellzey, Angus Pearson and F. A. Matsen, "Algebraic Formulation of Crystal Field Theory." The algebraic formulation which has developed for permutation group theory has been found to be applicable to crystal field theory. It is capable of reproducing all of the results of matrix representation theory and has, in addition, certain pedagogical advantages.
7. R. D. Poshusta and F. A. Matsen, "Finite Group Algebra and Quantum Mechanics." To be submitted to Volume III, THEORIE DES GROUPES EN PHYSIQUE CLASSIQUE ET QUANTIQUE, Theo Kahan, editor. The algebraic formulation of the

permutation group is here placed in a more sophisticated mathematical setting. In particular, the development has been tied into the theory of rings. The results obtained are essentially the same as those obtained in the technical report with the same name.

WORK IN PROGRESS

The true mass study of the helium atom is being vigorously extended and the results for the $2^3P$ states are about 1/3 completed.

A continuation of the computation of the integrals needed for a study of the lithium atom iso-electronic sequence is proceeding slowly due to the considerable difficulties involved.

Exploratory study has been begun on the peculiar problems associated with property and simply describing negative ions.

The work on the perturbation approach to elucidating atomic structure has unfortunately been almost completely halted due to a lack of available personnel.

WORK TERMINATED

Dr. H. Williamson has accepted a position with United Aircraft, Hartford, Connecticut, and is continuing the work on electron cross sections there. We have terminated all of our work in this area.